Air Products and Chemicals, Inc.
7201 Hamilton Boulevard
Allentown, PA 18195-1501
Telephone (610) 481-4911

28 December 2001

Via Certified US Mail and e-mail

Hon. Christine Todd Whitman
US Environmental Protection Agency
PO Box 1473
Merrifield, VA 22116

Attn: Chemical Right-to-Know Program

RE: Data Analysis, Test Plan and Robust Summaries for 2,4,7,9-tetramethyl-5-decyne-4,7-diol (CAS # 126-86-3).

Dear Ms. Whitman:

Air Products and Chemicals, Inc. is pleased to submit the attached data analysis and test plan for 2,4,7,9-tetramethyl-5-decyne-4,7-diol (CAS # 126-86-3) under the U.S. High Production Volume (HPV) Challenge Program. Also attached are robust summaries of the data in a IUCLID-format document.

This submission is also being sent electronically to the following e-mail addresses:

oppt.ncic@epa.gov
chem.rtk@epa.gov

Please contact me at (610) 481-2739 or by e-mail at hamiltce@apci.com if you have questions or if you require additional information.

Regards,

Carrie Hamilton
Toxicology Coordinator
Air Products and Chemicals, Inc.

2 Enclosures

cc w/o attachments: Charles Auer, Director, Chemical Control Division, U.S. EPA
Jim Keith, American Chemistry Council
Charles Bartish, Air Products and Chemicals, Inc.
Bronek Drozdowicz, Air Products and Chemicals, Inc.
Julie O'Brien, Air Products and Chemicals, Inc.

AR201-13452A

High Production Volume (HPV) Challenge Program

Data Analysis and Test Plan

For

2,4,7,9-Tetramethyl-5-decyne-4,7-diol

Prepared by:

Air Products and Chemicals, Inc.
7201 Hamilton Boulevard
Allentown, PA 18195

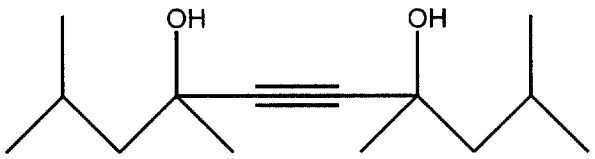
December 2001

Table of Contents

LIST OF TABLES

1.0 INTRODUCTION

2,4,7,9-Tetramethyl-5-decyne-4,7-diol is an acetylenic diol derived from acetylene and ketone and is used as a surfactant, defoamer, and wetting agent. 2,4,7,9-Tetramethyl-5-decyne-4,7-diol has the following structure:



Air Products and Chemicals, Inc. has committed to provide basic chemistry, environmental fate, ecotoxicity and health effects information on 2,4,7,9-Tetramethyl-5-decyne-4,7-diol (CAS 126-86-3) listed under the Environmental Protection Agency (EPA) High Production Volume (HPV) Chemical Challenge Program. By participating in this voluntary program, Air Products and Chemicals, Inc., agreed to assess the adequacy of existing data; prepare summaries of the data characterizing the chemical; determine data needed to fulfill the HPV data requirements; and design and submit a test plan to satisfy these testing requirements.

2.0 EVALUATION OF DATA

2.1 Physico-chemical Data

2.1.1 Melting Point: 54-55° C (129-131° F) [Ref. 1]

2.1.2 Boiling Point: 262-263° C (504-505° F) [Ref. 2]

2.1.3 Vapor Pressure: 0.66 ± 0.04 Pa @ 20°C ($4.9 \pm 0.3 \times 10^{-3}$ mm Hg) [Ref. 3]

2.1.4 Partition Coefficient: log Pow = 2.8 at 22-22.5 °C [Ref. 4]

2.1.5 Water Solubility: 1.70 g/l at 20±0.5 °C [Ref. 5]

2.1.6 Summary of Physico-chemical Data

Scientifically reliable data exists for all SIDS physico-chemical endpoints. No additional testing is recommended.

2.2 Environmental Fate and Biodegradation Data

2.2.1 Photodegradation:

Estimation Programs Interface for Microsoft® Windows (EPIWIN V3.05, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, Washington, D.C.), Atmospheric Oxidation Program (v1.90) modeling component was used to calculate the rate of photodegradation for 2,4,7,9-Tetramethyl-5-decyne-4,7-diol. The half-life was calculated to be 0.3 days (or 3 hours), assuming the reaction occurred over a 12-hour day with an average atmospheric concentration of 1.5×10^6 OH/cm^3 [Ref. 6].

2.2.2 Hydrolysis:

The half-life of 2,4,7,9-Tetramethyl-5-decyne-4,7-diol at pHs of 4, 7, and 9 is greater than one year at 25° C (OECD 111). 2,4,7,9-Tetramethyl-5-decyne-4,7-diol is hydrolytically stable [Ref. 7].

2.2.3 Biodegradation:

2,4,7,9-Tetramethyl-5-decyne-4,7-diol is not inhibitory towards biomass. In an activated sludge respiratory inhibition test (OECD 209) the 3-hr EC50 was approximately 680 ppm. [Ref. 8] 2,4,7,9-Tetramethyl-5-decyne-4,7-diol degraded approximately 5% in the Modified Sturm test (OECD 301B). 2,4,7,9-Tetramethyl-5-decyne-4,7-diol reached a daily degradation of approximately 25% (last 16 day daily average) in the Semi-Continuous Activated Sludge test (OECD 302A). These tests indicate that 2,4,7,9-Tetramethyl-5-decyne-4,7-diol is not readily biodegradable but it is inherently biodegradable [Ref. 9 and 10, respectively].

2.2.4 Transport/Distribution:

The LEV3EPI fugacity model (from EPIWIN V3.05, USEPA) was used for predicting partitioning of 2,4,7,9-Tetramethyl-5-decyne-4,7-diol among air, water, soil and sediment compartments. The following are the concentration results using a soil K_{oc} of 1,670 as calculated by the model and a log K_{ow} of 3.61 as calculated by the KOWWIN (USEPA) program [Ref. 11]:

- Air 0.4%
- Water 29%
- Soil 69%
- Sediment 2%

2.2.5 Summary of Environmental Fate and Biodegradation Data

Scientifically reliable data exists for all SIDS environmental fate and biodegradation endpoints. No additional testing is recommended.

2.3 Ecotoxicology Data

2.3.1 Acute Toxicity to Fish:

2,4,7,9-Tetramethyl-5-decyne-4,7-diol was tested in both fathead minnows and carp according to OECD guideline 203.

Fathead minnows (*Pimephales promelas*) were exposed for 96 hours to concentrations of 0, 4, 8, 16, 32, and 64 mg/l of 2,4,7,9-Tetramethyl-5-decyne-4,7-diol in a semi-static system. The 24- and 96-hour LC_{50} values (concentration causing 50% of the fish to die) were determined. All LC_{50} values were the same due to the fact that all deaths occurred within the first 24 hours of the test. The LC_{50} value for 24- and 96-hours was 36 mg/l with 95 percent confidence intervals ranging from 31 to 41 mg/l. [Ref. 12]

Carp (*Cyprinus carpio*) were exposed for 96 hours to concentrations of 0, 10, 18, 32, 56 and 100 mg/l of 2,4,7,9-Tetramethyl-5-decyne-4,7-diol in a static system. The 24- and 96-hour LC_{50} values were determined. All deaths occurred within the first 24 hours of the test. The LC_{50} value for 24- and 96- hours was 42 mg/l with 0 percent mortality at 32 mg/l and 100 percent mortality at 56 mg/l. Concentrations down to 18 mg/l induced effects on swimming behavior and pigmentation, while no sub-lethal effects occurred at 10 mg/l. The 96-hour No Observed Effect Level (NOEL) was 10 mg/l. [Ref. 13]

These results indicate that 2,4,7,9-Tetramethyl-5-decyne-4,7-diol is harmful to fish.

2.3.2 Acute Toxicity to Aquatic Invertebrates:

Daphnia magna were exposed for 24 hours to concentrations of 0, 62.5, 125, 250, 500, and 1000 mg/l. Four groups of 5 daphnia were exposed at each concentration. After 24 hours the number of immobilized Daphnia were counted. The 24-hour EC_{50} value (concentration causing 50% of the daphnia to be immobilized) was determined. The 24-hour EC_{50} was 88 mg/l. The confidence interval could not be calculated due to the lack of partial mortality in at least one concentration. However, this confidence interval would be expected to fall within 62.5 and 125 ppm, which are the chemical concentrations above and below the calculated EC_{50}. [Ref. 14]

Daphnia magna were exposed for 48 hours to concentrations of 0, 18, 32, 45, 100, and 180 mg/l. Two groups of 10 daphnia were exposed at each concentration. After 24 and 48 hours the number of immobilized Daphnia were counted and the 24- and 48-hour EC_{50} values were determined. OECD guideline 202 was followed. The 24-hour EC_{50} for Daphnia magna exposed to 2,4,7,9-Tetramethyl-5-decyne-4,7-diol was 99 mg/l based on average exposure concentrations with a 95 percent confidence interval between 83 and 130 mg/l. The 24-hour EC_{50} was 91 mg/l with a 95 percent confidence interval between 81 and 110 mg/l. The 48-hour No Observed Effect Concentration (NOEC) was 43 mg/l. [Ref. 15]

These results indicate that 2,4,7,9-Tetramethyl-5-decyne-4,7-diol is harmful to aquatic invertebrates.

2.3.3 Toxicity to Aquatic Plants:

Fresh water green algae (*Selenastrum capricornutum*) were examined in a 3-day growth inhibition test. Algal cultures were exposed to 2,4,7,9-Tetramethyl-5-decyne-4,7-diol in concentrations ranging from 1 to 100 mg/l, increasing with a factor of 2.2. The mean cell growth and the mean growth rate from each culture were calculated, and the EC_{50} values (concentration causing 50% reduction in biomass or growth rate) were determined. OECD guideline 201 was followed. The 72-hour EC_{50} for algal cell growth inhibition (E_BC_{50}) was 15 mg/l with a 95 % confidence interval ranging from 9 to 23 mg/l. The EC_{50} for algal cell growth rate reduction (E_RC_{50}: 0-72h) was 82 mg/l with a 95 % confidence interval ranging from 39 to 170 mg/l. The NOEC for algal cell growth inhibition and growth rate reduction was 1.0 mg/l. However, a recovery of growth was observed during the last 48 hours of exposure with a NOEC of 4.6 mg/l for growth rate. [Ref. 16]

These results indicate that 2,4,7,9-Tetramethyl-5-decyne-4,7-diol is harmful to algae.

2.3.4 Summary of Ecotoxicology Data

2,4,7,9-Tetramethyl-5-decyne-4,7-diol is harmful to fish, daphnia and algae. Scientifically reliable data exists for all SIDS ecotoxicity endpoints. No additional ecotoxicity testing is recommended.

2.4 Health Effects Data

2.4.1 Acute Health Effects

2.4.1.1 Acute Oral Toxicity

Ten Sprague-Dawley rats were orally administered 2,4,7,9-Tetramethyl-5-decyne-4,7-diol. The 2,4,7,9-Tetramethyl-5-decyne-4,7-diol was prepared as a 5% solution in hydrous alcohol. Each rat received a dose volume of 10 ml/kg of body weight. The animals were observed daily post-dose for 14 days. All animals survived, showed no abnormal clinical signs and gained weight. Gross necropsy did not reveal any test material-related pathological changes. The oral LD_{50} for 2,4,7,9-Tetramethyl-5-decyne-4,7-diol in rats was greater than 500 mg/kg. [Ref. 17]

2.4.1.2 Acute Inhalation Toxicity

Ten rats were exposed to 2,4,7,9-Tetramethyl-5-decyne-4,7-diol via inhalation. The 2,4,7,9-Tetramethyl-5-decyne-4,7-diol was prepared as a 5% aqueous solution. The test solution was aerosolized to provide a concentration of greater than 20 mg of mist per liter of chamber air over the one-hour period. The test atmosphere was not analyzed. The animals were observed daily for 14 days. All animals survived. Ocular and nasal irritation as well as a reduction in spontaneous activity was noted in all animals immediately following the one-hour exposure. All animals returned to normal within 3 hours. One male and one female were autopsied at random. Gross necropsy did not reveal any test material-related pathological changes. The inhalation LC_{50} for 2,4,7,9-Tetramethyl-5-decyne-4,7-diol in rats was greater than 20 mg/l. [Ref. 18]

2.4.1.3 Acute Dermal Toxicity

Six New Zealand White rabbits were exposed dermally to 2,4,7,9-Tetramethyl-5-decyne-4,7-diol. The neat 2,4,7,9-Tetramethyl-5-decyne-4,7-diol (1,000 mg/kg) was applied to an intact shaved skin site. The entire trunk of each animal was then encased in a plastic sleeve to ensure continuous contact of the test material with the skin for a 24-hour period. The sleeve was removed after 24 hours and the animals were observed daily for 14 days. No dermal erythema or edema was seen in any animal during the 14-day observation period. There was no mortality. The dermal LD_{50} for 2,4,7,9-Tetramethyl-5-decyne-4,7-diol in rabbits was greater than 1,000 mg/kg. [Ref. 19]

Five rats of each sex were administered 2,000 mg/kg of 2,4,7,9-Tetramethyl-5-decyne-4,7-diol by dermal application. OECD guideline 402 was followed. No mortality and no clinical signs of ill health were observed during the study. Skin abnormalities on the treated area included scales and

scabs in two females between days 4 and 6. Low body weight gain or body weight loss was noted in all animals over the first week of the study with improved body weight gain over the second week. Macroscopic post mortem examination of the animals at termination did not reveal any significant abnormalities. The dermal LD_{50} for 2,4,7,9-Tetramethyl-5-decyne-4,7-diol in rats was greater than 2,000 mg/kg. [Ref. 20]

2.4.1.4 Summary of Acute Toxicological Effects

2,4,7,9-Tetramethyl-5-decyne-4,7-diol is practically non-toxic following a single oral, inhalation, or dermal exposure. Scientifically reliable data exists for all SIDS acute toxicity endpoints. No additional acute toxicity testing is recommended.

2.4.2 Genetic Toxicology Effects

2.4.2.1 Bacterial Gene Mutation Assay

2,4,7,9-Tetramethyl-5-decyne-4,7-diol diluted in dimethylsulfoxide (DMSO) was examined for mutagenic activity in the Salmonella-Escherichia coli/microsome plate incorporation assay. OECD guidelines were followed. The assay was performed using the standard plate incorporation procedure with *S. typhimurium* strains TA1535, TA1537, TA98, and TA100 and *E. coli* strain WP2 (uvrA) over a dose range of 10 to 5,000 ug/plate in both the presence and absence of an Aroclor 1254-induced rat-liver metabolic activation system. The initial experiment used 5 percent (v/v) metabolic activation and the repeat experiment used 10 percent (v/v) metabolic activation. 2,4,7,9-Tetramethyl-5-decyne-4,7-diol was not mutagenic under the test conditions used in this bacterial assay. [Ref. 21]

2.4.2.2 *In Vitro* Chromosomal Aberration Assay

2,4,7,9-Tetramethyl-5-decyne-4,7-diol was tested for its ability to induce chromosome aberrations in Chinese hamster ovary (CHO) cells in the presence and absence of rat S-9 metabolic activation (MA) according to OECD guideline 473.

In the preliminary cytotoxicity assay, CHO cells were exposed to 2,4,7,9-Tetramethyl-5-decyne-4,7-diol at concentrations of 19.5, 78.3, 312.5, 1250, and 3500 mg/ml in both the absence and presence of MA. A high dose of 3500 mg/ml was used based on the limit of solubility of the test article in DMSO. Cells were exposed to the test article in the absence of MA for 3 and 21 hours and in the presence of MA for 3 hours. At 21 hours after exposure initiation, cells were harvested and evaluated. All of the cultures from the top two dose levels exhibited a significant decrease in confluency (0 to 25 percent) and therefore were not harvested. For cultures exposed to the test article for 3 hours in the presence or absence of MA, no significant reduction in mitotic index was observed at dose levels of 312.5 mg/ml and below. Cultures exposed for 21 hours to the test article at 312.5 mg/ml showed a significant reduction in mitotic index.

Based on the cytotoxicity results, the initial chromosome aberration study was performed by exposing CHO cells for 3 hours to 2,4,7,9-Tetramethyl-5-decyne-4,7-diol at concentrations of 19.5, 39.1, 78.1, 156.3, and 312.5 mg/ml in both the absence and presence of MA. At 21 hours after initiation of exposure, cells were harvested and evaluated. Cytotoxicity was evident in cultures exposed to 312.5 mg/ml both with and without MA, so the cells were not harvested for evaluation. In cultures at the three dose levels scored (39.1, 78.1, and 156.3 mg/ml), there was no statistically significant increase in the number of cells with structural aberrations and the mitotic index was comparable to that for the control. No increases in polyploidy were observed in the presence or absence of MA.

The dose levels for the replicate experiment were based on the results of the cytotoxicity experiment (-MA) and the initial experiment (+MA), which indicated cytotoxicity and a significant reduction in confluency at the 312.5-mg/ml dose level. The replicate experiment was performed by exposing

CHO cells for 21 hours to the test article at concentrations of 9.8, 19.5, 39.1, 78.1, and 156.3 mg/ml in the absence of MA, and for 3 hours at concentrations of 19.5, 39.1, 78.1, and 156.3 mg/ml in the presence of MA. At 21 hours after initiation of exposure, cells were harvested and evaluated. At the three dose levels scored in both MA conditions (39.1, 78.1, and 156.3 mg/ml), there was no statistically significant increase in the number of cells with structural aberrations and the mitotic index was comparable to that for the control. No increases in polyploidy were observed in the presence or absence of MA. 2,4,7,9-Tetramethyl-5-decyne-4,7-diol did not induce structural chromosome damage in this in vitro CHO cell system. [Ref. 22]

2.4.2.3 Summary of Genetic Toxicology Effects

2,4,7,9-Tetramethyl-5-decyne-4,7-diol was not mutagenic when examined in an *in vitro* bacterial assay and was not clastogenic when examined in an *in vitro* mammalian cell assay. Scientifically reliable data exists for all SIDS genetic toxicity endpoints. No additional genetic toxicity testing is recommended.

2.4.3 Repeated Dose Health Effects

2.4.3.1 Systemic Oral Toxicity

2,4,7,9-Tetramethyl-5-decyne-4,7-diol was administered in the diet to groups of male and female Long-Evans rats for 28 days. Each group was composed of 6 rats of each sex. The rats were approximately 6-7 weeks of age at the start of the test. The dose levels were 0, 625, 1250, 2500, and 5000 ppm. Test diets were made up on a weekly basis. Statistical analysis of the body weight and food consumption data was performed using the F-test and the Student's t-test. Mortality, physical observations, body weight, and food consumption data, as well as gross necropsy observations did not reveal any adverse effects considered to be attributable to the administration of 2,4,7,9-Tetramethyl-5-decyne-4,7-diol at any of the dose levels. The NOEL was 5000 ppm. [Ref. 23]

In a repeated dose oral toxicity study, groups of four male and four female beagle dogs were administered 2,4,7,9-Tetramethyl-5-decyne-4,7-diol in gelatin capsules at dose levels of 0, 200, 250 and 300 mg/kg/day for 91 days. Because the dogs had to be gradually acclimated from 50 mg/kg/day to higher dose levels of 2,4,7,9-Tetramethyl-5-decyne-4,7-diol to avoid vomiting, the total test period was 130 days. The control animals received capsules of granulated table sugar. Capsule administration followed feeding by approximately one hour.

All dogs survived for the duration of this study with few clinical signs. Occasional dogs in the mid- and high-dose groups exhibited sporadic, neurological disturbances (convulsions, tremors) during the study. All other observations, including feed consumption, body weight gains, organ weights (except liver), clinical chemistries, hematology, urinalysis, gross pathology, and histology were judged to reflect no compound-related or biologically significant changes.

This study did not establish a NOEL for 2,4,7,9-Tetramethyl-5-decyne-4,7-diol in dogs, since mean liver weights and liver-to-body weight ratios in all treated groups were higher than in the corresponding control groups. However, since no histological abnormalities were observed in these livers, the liver enlargement was judged to be due to hyperplasia of the hepatic endoplasmic reticulum, where xenobiotic/drug metabolizing enzymes are located. [Ref. 24]

2.4.3.2 Reproductive and Developmental Toxicity

2,4,7,9-Tetramethyl-5-decyne-4,7-diol was administered to rats during a single generation reproduction study and for ninety one days to the F1a weanlings. The test material was mixed into the rats' feed to provide dose levels of 0, 500, 1000, and 2000 mg/kg/day.

Sexually mature Sprague-Dawley albino rats were divided into four groups, each consisting of ten male and twenty female rats. All Fo male rats, both test and control, were fed their respective diets

until their litters reached the age of 21 days for weaning, when the Fo dams were sacrificed. The weanlings were randomized to their respective groups and carried on the same dose levels to the termination of the experiment.

The only pertinent findings observed in the Fo parents were: decreased body weight and feed consumption of the high-dose female group, slight decrease in the mean weaning weight of both male and female pups of the high-dose group, and a slight decrease in the lactation indices of the high-dose group. Histology of the reproductive organs in the Fo parents revealed no abnormalities.

A slight decrease in the mean rate of body weight gain was observed in the mid- and high-dose F1a male and female rats; there was also a significant decrease in this parameter in the low-dose male group during the first eight weeks. All groups exhibited normal mean hematological, clinical chemistry, and urinalysis findings after 91 days on test. The mid- and high-dose groups exhibited a significant increase in their absolute and relative liver weights. Histopathology of the liver of the mid- and high-dose F1a male and female rats showed mild to moderate centrilobular cloudy swelling of the hepatocytes.

2,4,7,9-Tetramethyl-5-decyne-4,7-diol, when fed to rats under the conditions of this experiment, showed no effect at 500 mg/kg/day but did have a toxic effect in the F1a generation at greater than or equal to 1,000 mg/kg/day while in the reproduction phase of this experiment there was a toxic effect at the 2,000 mg/kg/day level, a borderline effect at the 1,000 mg/kg/day level and no effect at 500 mg/kg/day. [Ref. 25]

2.4.3.3 Summary of Systemic, Reproductive and Developmental Toxicity Effects

Effects on the reproductive organs were assessed in all of the repeated dose studies summarized above. There were no adverse effects on the reproductive organs in males and females examined grossly or histologically at doses up to and including 300 mg/kg in dogs and 2,000 mg/kg in rats.

Repeat-dose studies in rats and dogs showed few effects. A mild effect on the liver was seen in both species.

All of the repeat-dose studies are scientifically reliable. No further testing for systemic, reproductive or developmental effects is recommended.

3.0 CONCLUSIONS

All of the data needed to meet the requirements of the HPV program are available and of high quality. No further studies or data are needed to assess the hazards of 2,4,7,9-Tetramethyl-5-decyne-4,7-diol. Table 1 shows the studies that exist for 2,4,7,9-Tetramethyl-5-decyne-4,7-diol.

TABLE 1: HPV DATA REQUIREMENTS/CRITICAL STUDIES: 2,4,7,9-Tetramethyl-5-decyne-4,7-diol

HPV Data Category	Test Endpoint		Acceptable Data Reference (Klimisch Rating)	Data to be Generated
Physical and Chemical Properties	Melting Point		1 (1)	No
	Boiling Point		2 (1)	No
	Vapor Pressure		3 (1)	No
	Partition Coefficient		4 (1)	No
	Water Solubility		5 (1)	No
Environmental Fate and Pathways	Photodegradation		6 (2)	No
	Hydrolysis		7 (1)	No
	Biodegradation		8 (1), 9 (1), 10 (1)	No
	Transport/Distribution		11 (2)	No
Ecotoxicity	Acute toxicity to Fish		12 (2), 13 (1)	No
	Acute toxicity to Aquatic Invertebrates		14 (2), 15 (1)	No
	Toxicity to Aquatic Plants		16 (1)	No
	Chronic aquatic invertebrate test[1]		NR	No
	Terrestrial toxicity[1]		NR	No
Human Health Effects	Acute toxicity		17 (2), 18 (2), 19 (2), 20 (1)	No
	Repeated Dose		23 (2), 24 (2)	No
	Genetic Toxicity	Gene Mutation	21 (1)	No
		Chromosome Aberration	22 (1)	No
	Reproductive Toxicity		25 (2)	No
	Developmental Toxicity		25 (2)	No

Notes:
Data listed are cross-referenced to a Robust Summary report [i.e. 1 (2)]; which identifies the reference number and Klimisch Rating ( ). If more than one study is listed it means they are co-critical.

[1] = Test are not required for all chemicals; only when appropriate.

NR = Not Required

4.0 REFERENCES

1. Melting Point: Air Products and Chemicals, Inc. (EXT-99/084). 2,4,7,9-Tetramethyl-5-decyne-4,7-diol: Determination of the Melting Temperature (OECD 102). Testing Facility: NOTOX B.V., 's-Hertogenbosch, The Netherlands. Study year: 1999. Klimisch = 1

2. Boiling Point: Air Products and Chemicals, Inc. (EXT-99/083). 2,4,7,9-Tetramethyl-5-decyne-4,7-diol: Determination of the Boiling Temperature (OECD 103). Testing Facility: NOTOX B.V., 's-Hertogenbosch, The Netherlands. Study year: 1999. Klimisch = 1

3. Vapor Pressure: Air Products and Chemicals, Inc. (EXT-99/082). 2,4,7,9-Tetramethyl-5-decyne-4,7-diol: Determination of the Vapor Pressure (OECD 104). Testing Facility: NOTOX B.V., 's-Hertogenbosch, The Netherlands. Study year: 1999. Klimisch = 1

4. Partition Coefficient: Air Products and Chemicals, Inc. (EXT-99/100). 2,4,7,9-Tetramethyl-5-decyne-4,7-diol: Determination of the Partition Coefficient (N-Octanol/Water) (OECD 117). Testing Facility: NOTOX B.V., 's-Hertogenbosch, The Netherlands. Study year: 1999. Klimisch = 1

5. Water Solubility: Air Products and Chemicals, Inc. (EXT-99/099). 2,4,7,9-Tetramethyl-5-decyne-4,7-diol: Determination of the Water Solubility (OECD 105). Testing Facility: NOTOX B.V., 's-Hertogenbosch, The Netherlands. Study year: 1999. Klimisch = 1

6. Photodegradation: Estimation Programs Interface for Microsoft® Windows (EPIWIN V3.05, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, Washington, D.C.) Atmospheric Oxidation Program (v1.90). Klimisch = 2

7. Hydrolysis: Air Products and Chemicals, Inc. (EXT-00/001). 2,4,7,9-Tetramethyl-5-decyne-4,7-diol: Determination of the Hydrolysis as a Function of pH (OECD 111). Testing Facility: NOTOX B.V., 's-Hertogenbosch, The Netherlands. Study year: 2000. Klimisch = 1

8. Biodegradation: Air Products and Chemicals, Inc. (PFT-99/004). Activated Sludge, Respiration Inhibition Testing, OECD 209 for Surfynol 104 Surfactant. Testing Facility: SGS U.S. Testing Company Inc., Fairfield, New Jersey, USA. Study year: 1999. Klimisch = 1

9. Biodegradation: Air Products and Chemicals, Inc. (EXT-99/097). 2,4,7,9-Tetramethyl-5-decyne-4,7-diol: Determination of "Ready" Biodegradability: Carbon Dioxide (CO2) Evolution Test (Modified Sturm Test) (OECD 301B). Testing Facility: NOTOX B.V., 's-Hertogenbosch, The Netherlands. Study year: 1999. Klimisch = 1

10. Biodegradation: Air Products and Chemicals, Inc. (PFT-99/004). Semi-Continuous Activated Sludge Test (OECD Method 302A) for Surfynol 104 Surfactant. Testing Facility: SGS U.S. Testing Company Inc., Fairfield, New Jersey, USA. Study year: 1999. Klimisch = 1

11. Transport/Distribution: Estimation Programs Interface for Microsoft® Windows (EPIWIN V3.05, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, Washington, D.C.) LEV3EPI Fugacity Model. Klimisch = 2

12. Acute Toxicity to Fish: Air Products and Chemicals, Inc. (EXT-92/040). Surfynol 104 Fish Toxicity Results. Testing Facility: Commonwealth Technology, Inc., Lexington, Kentucky, USA . Study year: 1991. Klimisch = 2

13. Acute Toxicity to Fish: Air Products and Chemicals, Inc. (EXT-00/007). 2,4,7,9-Tetramethyl-5-decyne-4,7-diol (Static): 96-Hour Acute Toxicity Study In Carp (OECD 203). Testing Facility: NOTOX B.V., 's-Hertogenbosch, The Netherlands. Study year: 2000. Klimisch = 1

14. Acute Toxicity to Aquatic Invertebrates: Air Products and Chemicals, Inc. (EXT-92/040). Surfynol 104 Fish Toxicity Results. Testing Facility: Commonwealth Technology, Inc., Lexington, Kentucky, USA. Study year: 1991. Klimisch = 2

15. Acute Toxicity to Aquatic Invertebrates: Air Products and Chemicals, Inc. (EXT-99/101). 2,4,7,9-Tetramethyl-5-decyne-4,7-diol: Acute Static Toxicity Study In Daphnia Magna (OECD 202, Part 1). Testing Facility: NOTOX B.V., 's-Hertogenbosch, The Netherlands. Study year: 2000. Klimisch = 1

16. Toxicity to Aquatic Plants: Air Products and Chemicals, Inc. (EXT-00/030). 2,4,7,9-Tetramethyl-5-decyne-4,7-diol: Fresh Water Algal Growth Inhibition Test (OECD 201). Testing Facility: NOTOX B.V., 's-Hertogenbosch, The Netherlands. Study year: 2000. Klimisch = 1

17. Acute Oral Toxicity: Air Products and Chemicals, Inc. (EXT-86/020). 2,4,7,9-Tetramethyl-5-decyne-4,7-diol: Acute Toxicity Studies. Testing Facility: Foster D. Snell Biological Sciences Laboratory, Elizabeth, New Jersey, USA. Study year: 1971. Klimisch = 2

18. Acute Inhalation Toxicity: Air Products and Chemicals, Inc. (EXT-86/020). 2,4,7,9-Tetramethyl-5-decyne-4,7-diol: Acute Toxicity Studies. Testing Facility: Foster D. Snell Biological Sciences Laboratory, Elizabeth, New Jersey, USA. Study year: 1971. Klimisch = 2

19. Acute Dermal Toxicity: Air Products and Chemicals, Inc. (EXT-86/020). 2,4,7,9-Tetramethyl-5-decyne-4,7-diol: Acute Toxicity Studies. Testing Facility: Foster D. Snell Biological Sciences Laboratory, Elizabeth, New Jersey, USA. Study year: 1971. Klimisch = 2

20. Acute Dermal Toxicity: Air Products and Chemicals, Inc. (EXT-94/012). Assessment of Acute Dermal Toxicity with Surfynol 104 in the Rat. Testing Facility: NOTOX B.V., 's-Hertogenbosch, The Netherlands. Study year: 1993. Klimisch = 1

21. Gene Mutation: Air Products and Chemicals, Inc. (EXT-99/078). Evaluation of 2,4,7,9-Tetramethyl-5-decyne-4,7-diol in the Salmonella-Escherichia Coli/Microsome Plate Incorporation Assay (OECD 471). Testing Facility: SRI International Toxicology Laboratory, Menlo Park, California, USA. Study year: 1999. Klimisch = 1

22. Chromosome Aberration: Air Products and Chemicals, Inc. (EXT-99/091). Evaluation of 2,4,7,9-Tetramethyl-5-decyne-4,7-diol in the CHO Chromosome Aberration Assay (OECD 473). Testing Facility: SRI International Toxicology Laboratory, Menlo Park, California, USA. Study year: 1999. Klimisch = 1

23. Systemic Oral Toxicity: Air Products and Chemicals, Inc. (EXT-77/016). A Four-Week Dose Range-Finding Study of Surfynol-104 In Rats. Testing Facility: Bio/dynamics Inc., East Millstone, New Jersey, USA. Study year: 1977. Klimisch = 2

24. Systemic Oral Toxicity: Air Products and Chemicals, Inc. (EXT-94/090). Surfynol 104 - Modified 91-Day Feeding Study In The Dog. Testing Facility: Pharmacopathics Research Laboratories, Laurel, Maryland, USA. Study year: 1979. Klimisch = 2

25. Reproductive and Developmental Toxicity: Air Products and Chemicals, Inc. (EXT-97/005). Surfynol 104: I. Single Generation Reproduction Study in the Rat (Fo-F1a). II. 91-Day Feeding Study (F1a Rats). Testing Facility: Pharmacopathics Research Laboratories, Laurel, Maryland, USA. Study year: 1979. Klimisch = 2

AR201-13452B

IUCLID

Data Set

New Chemical	:	ID: 126-86-3
CAS No.	:	126-86-3
EINECS Name	:	2,4,7,9-Tetramethyl-5-decyne-4,7-diol
EINECS No.	:	204-809-1
Structural Formula	:	CC(CC(O)(C)C#CC(C)(CC(C)C)O)C

Producer Related Part

Company	:	Air Products and Chemicals, Inc.
Creation date	:	20.09.1999

Substance Related Part

Company	:	Air Products and Chemicals, Inc.
Creation date	:	20.09.1999

Memo	:	
Printing date	:	18.12.2001
Revision date	:	
Date of last Update	:	13.12.2001
Number of Pages	:	25
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 7
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 OECD AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE

1.0.3 IDENTITY OF RECIPIENTS

1.1 GENERAL SUBSTANCE INFORMATION

Substance type : organic
Physical status : solid
Purity : >= 98 % w/w
20.09.1999

1.1.0 DETAILS ON TEMPLATE

1.1.1 SPECTRA

1.2 SYNONYMS

1,4-Diisobutyl-1,4-dimethylbutynediol
20.09.1999

2,4,7,9-Tetramethyl-5-decyne-4,7-diol (ENCS, ECL)
20.09.1999

2,4,7,9-Tetramethyldec-5-in-4,7-diol (German) (EINECS)
20.09.1999

2,4,7,9-Tetramethyldec-5-yne-4,7-diol (English, French) (DSL, EINECS)
20.09.1999

5-Decyne-4,7-diol, 2,4,7,9-tetramethyl- (TSCA, DSL, AICS)
20.09.1999

Surfynol 104
20.09.1999

1.3 IMPURITIES

CAS-No : 7732-18-5
EINECS-No :
EINECS-Name : Water
Contents : <= 2 % w/w
20.09.1999

CAS-No	:	108-10-1
EINECS-No	:	203-550-1
EINECS-Name	:	4-methylpentane-2-one
Contents	:	<= 0.54 % w/w

13.12.2001

CAS-No	:	
EINECS-No	:	
EINECS-Name	:	Dimethyl Hexynol
Contents	:	<= 0.54 % w/w

13.12.2001

1.4 ADDITIVES

1.5 QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.7 USE PATTERN

1.7.1 TECHNOLOGY PRODUCTION/USE

Type	:	Use
Remark	:	Uses of 2,4,7,9-tetramethyl-5-decyne-4,7-diol

There are two major direct uses for 2,4,7,9-tetramethyl-5-decyne-4,7-diol (CAS # 126-86-3). Most of the 2,4,7,9-tetramethyl-5-decyne-4,7-diol manufactured is used as an industrial defoaming, nonionic surfactant. A lesser quantity of the product is consumed as a chemical intermediate and is converted into a polyethylene glycol ether surfactant, also for use in industrial applications.

2,4,7,9-tetramethyl-5-decyne-4,7-diol has been marketed for predominantly waterborne industrial applications in the coatings, ink, and adhesive industries. Though a critical contributor to the performance of a formulated product, the surfactant is generally applied in low use levels, typically 0.1 - 0.5%.

Due to its ability to reduce surface tension under dynamic conditions, 2,4,7,9-tetramethyl-5-decyne-4,7-diol surfactant is used to enhance wetting of oily or improperly cleaned substrates and to improve coverage over low surface tension substrates like plastic in waterborne architectural, industrial maintenance, general industrial, wood, plastic, concrete and paper coatings.

The 2,4,7,9-tetramethyl-5-decyne-4,7-diol surfactant is also employed for its multifunctional benefits in water-based printing inks. The product aids in penetration of the ink into absorbent stocks such as paper and also improves coverage over polymeric films such as polyethylene. In addition, the surfactant's unique capabilities eliminate foam, which causes many problems in printing inks. In overprint varnish systems, the surfactant provides wetting so that proper coverage of an aqueous overprint varnish can be achieved over wet solvent-based lithographic ink. The surfactant is also used in lithographic fountain solutions for the dynamic wetting of printing plates without causing excess emulsification of the ink. In pigment grinding applications, the surfactant provides good color development for maximum tint strength and lower viscosity dispersions for efficient grinding at higher pigment loadings.

2,4,7,9-tetramethyl-5-decyne-4,7-diol is used as a component of pressure sensitive adhesives, plywood adhesives, and laminating adhesives. The low surface tensions presented by silicone and plastic film release liners require strong wetting agents in order to achieve proper coverage by the adhesive.

The unique multifunctional properties of 2,4,7,9-tetramethyl-5-decyne-4,7-diol surfactant that make it successful in waterborne coatings, ink, and adhesive formulations also apply to several other applications. The following represent some of the other areas where our products are also used: industrial cleaners, agriculture, latex dipping, emulsion polymerization, foundry, metalworking fluids, and chemical processing.

In its other major use, some of the 2,4,7,9-tetramethyl-5-decyne-4,7-diol manufactured is converted to polyethylene glycol ether surfactants. These products represent a range of ethoxylation with varying water solubility, foaming and wetting characteristics.

13.12.2001

1.8 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.9 SOURCE OF EXPOSURE

1.10.1 RECOMMENDATIONS/PRECAUTIONARY MEASURES

1.10.2 EMERGENCY MEASURES

1.11 PACKAGING

1.12 POSSIB. OF RENDERING SUBST. HARMLESS

1.13 STATEMENTS CONCERNING WASTE

1.14.1 WATER POLLUTION

1.14.2 MAJOR ACCIDENT HAZARDS

1.14.3 AIR POLLUTION

1.15 ADDITIONAL REMARKS

1.16 LAST LITERATURE SEARCH

1.17 REVIEWS

1.18 LISTINGS E.G. CHEMICAL INVENTORIES

2.1 MELTING POINT

Value	:	= 54 - 55 ° C
Decomposition	:	no
Sublimation	:	no
Method	:	OECD Guide-line 102 "Melting Point/Melting Range"
Year	:	1999
GLP	:	yes
Test substance	:	

15.11.1999

2.2 BOILING POINT

Value	:	= 262 - 263 ° C
Decomposition	:	no
Method	:	OECD Guide-line 103 "Boiling Point/boiling Range"
Year	:	1999
GLP	:	yes
Test substance	:	
Remark	:	The measured boiling temperature depends on the atmospheric pressure. The determination of the correction factor to standard pressure is beyond the scope of this study. Therefore no correction was applied to the boiling temperature observed.

15.11.1999

2.3 DENSITY

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	= 0.62 - 0.7 hPa at 20° C
Decomposition	:	
Method		OECD Guide-line 104 "Vapour Pressure Curve"
Year	:	1999
GLP	:	yes
Test substance	:	

13.12.2001

2.5 PARTITION COEFFICIENT

Log pow	:	= 2.8 at 22° C
Method		OECD Guide-line 117 "Partition Coefficient (n-octanol/water), HPLC Method"
Year	:	1999

GLP	:	yes
Test substance	:	

16.12.1999

2.6.1 WATER SOLUBILITY

Value	:	= 1.7 g/l at 20 ° C
Qualitative	:	soluble (1000-10000 mg/L)
Pka	:	
PH	:	= 7.3 - 7.5
Method	:	OECD Guide-line 105 "Water Solubility"
Year	:	1999
GLP	:	yes
Test substance	:	

16.12.1999

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Deg. Product	:	
Method	:	other (calculated)
Year	:	2000
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	EPIWIN Suite (QSAR) Properties AOP Program (V1.87)
Result	:	Half-life equals 3.021 hours. Photodegrades rapidly in the atmosphere.

15.03.2000 (13)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	
t1/2 pH7	:	
t1/2 pH9	:	
Deg. Product	:	
Method	:	OECD Guide-line 111 "Hydrolysis as a Function of pH"
Year	:	2000
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	Half-life time at 25 degrees C greater than 1 year at pH 4, pH 7, and pH 9.
Reliability	:	(1) valid without restriction

15.03.2000 (1)

3.1.3 STABILITY IN SOIL

3.2 MONITORING DATA

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	
Media	:	
Air (level I)	:	
Water (level I)	:	
Soil (level I)	:	
Biota (level II / III)	:	
Soil (level II / III)	:	
Method	:	other
Year	:	2000
Method	:	EPIWIN Suite (QSAR) Properties. STP Fugacity Model; predicted fate in a wastewater treatment facility.
Result	:	Molecular weight (g/mol) 226.36 Aqueous solubility (mg/l) 1700

Vapour pressure (Pa) 0.65328
(atm) 6.44737E-006
(mm Hg) 0.0049
Henry 's law constant (Atm-m3/mol) 8.58483E-007
Air-water partition coefficient 3.51094E-005
Octanol-water partition coefficient (Kow) 630.957
Log Kow 2.8
Biomass to water partition coefficient 126.991
Temperature [deg C] 25
Biodeg rate constants (h^-1),half life in biomass (h) and in 2000 mg/L MLSS (h):

-Primary tank	0.00	2025.41	10000.00
-Aeration tank	0.00	2025.41	10000.00
-Settling tank	0.00	2025.41	10000.00

STP Overall Chemical Mass Balance:

	g/h	mol/h	percent
Influent	1.00E+001	4.4E-002	100.00
Primary sludge	1.72E-001	7.6E-004	1.72
Waste sludge	2.47E-001	1.1E-003	2.47
Primary volatilization	4.55E-004	2.0E-006	0.00
Settling volatilization	1.24E-003	5.5E-006	0.01
Aeration off gas	3.06E-003	1.4E-005	0.03
Primary biodegradation	2.15E-003	9.5E-006	0.02
Settling biodegradation	6.41E-004	2.8E-006	0.01
Aeration biodegradation	8.44E-003	3.7E-005	0.08
Final water effluent	9.56E+000	4.2E-002	95.65
Total removal	4.35E-001	1.9E-003	4.35
Total biodegradation	1.12E-002	5.0E-005	0.11

15.03.2000 (13)

Type :
Media :
Air (level I) :
Water (level I) :
Soil (level I) :
Biota (level II / III) :
Soil (level II / III) :
Method : other
Year : 2001
Method : EPIWIN V3.05 LEV3EPI Fugacity Model
Result : Level III Fugacity Model (Full-Output):

==========

Chem Name : 5-Decyne-4,7-diol, 2,4,7,9-tetramethyl-
Molecular Wt: 226.36
Henry's LC : 8.58e-007 atm-m3/mole (calc VP/Wsol)
Vapor Press : 0.0049 mm Hg (user-entered)
Liquid VP : 0.00959 mm Hg (super-cooled)
Melting Pt. : 54.5 deg C (user-entered)
Log Kow : 2.8 (user-entered)

Soil Koc : 259 (calc by model)

	Concentration (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.425	6.04	1000
Water	31.8	900	1000
Soil	67.4	900	1000
Sediment	0.383	3.6e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	8.53e-012	907	79.1	30.2	2.64
Water	1.12e-011	456	592	15.2	19.7
Soil	4.05e-011	964	0	32.1	0
Sediment	9.37e-012	1.37	0.142	0.0457	0.00475

Persistence Time: 620 hr
Reaction Time: 798 hr
Advection Time: 2.77e+003 hr
Percent Reacted: 77.6
Percent Advected: 22.4

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 6.039
Water: 900
Soil: 900
Sediment: 3600
Biowin estimate: 2.275 (weeks-months)

Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

13.12.2001

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type	:	aerobic
Inoculum	:	activated sludge, domestic
Contact time	:	
Degradation	:	= 5% after 28 day
Result	:	
Deg. Product	:	
Method	:	OECD Guide-line 301 B "Ready Biodegradability: Modified Sturm Test (CO_2 evolution)"
Year	:	1999
GLP	:	Yes
Test substance	:	as prescribed by 1.1 - 1.4

15.03.2000 (14)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	semistatic
Species	:	Pimephales promelas (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	No
LC50	:	= 36
Method	:	OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year	:	1991
GLP	:	No
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Fish measuring 2 cm +/- 1 cm at the start of test were exposed to Surfynol 104 at concentrations of 0, 4, 8, 16, 32, and 64 ppm. Two groups of 10 fish were exposed at each concentration. The dissolved oxygen, water pH, specific conductance, total hardness and total alkalinity were measured. All deaths occurred within the first 24 hours. Statistical analysis was performed using the Trimmed Spearman-Karber method. Information on fish age, and test temperature and lighting were not recorded.
Source	:	APCI (EXT-92/040) / Commonwealth Technology, Inc.
Reliability	:	(2) valid with restrictions

06.11.2001 (4)

Type	:	static
Species	:	Cyprinus carpio (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	yes
NOEC	:	= 10
LC0	:	= 32
LC50	:	= 42
LC100	:	= 56
Method	:	OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year	:	2000
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Reliability	:	(1) valid without restriction

14.06.2001 (11)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	static
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
Analytical monitoring	:	no
EC50	:	= 88
Method	:	OECD Guide-line 202, part 1 "Daphnia sp., Acute Immobilisation Test"
Year	:	1991
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Daphnia which were < 27 hours old at the start of test were exposed to Surfynol 104 at concentrations of 0, 62.5, 125, 250, 500, and 1000 ppm.

Four groups of 5 daphnia were exposed at each concentration. The dissolved oxygen, water pH, specific conductance, total hardness and total alkalinity were measured. Statistical analysis was performed using the Trimmed Spearman-Karber method. Information on test temperature and lighting were not recorded.

Source : APCI (EXT-92/040) / Commonwealth Technology, Inc.
Reliability : (2) valid with restrictions
06.11.2001 (4)

Type :
Species : Daphnia magna (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
Analytical monitoring : yes
NOEC : = 43
EC50 : = 91
Method : OECD Guide-line 202, part 1 "Daphnia sp., Acute Immobilisation Test"
Year : 2000
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Reliability : (1) valid without restriction
14.06.2001 (10)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species : Selenastrum capricornutum (Algae)
Endpoint : biomass
Exposure period : 72 hour(s)
Unit : mg/l
Analytical monitoring : yes
NOEC : = 1
EC10 : = 1.8
EC50 : = 15
Method : OECD Guide-line 201 "Algae, Growth Inhibition Test"
Year : 2000
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Result : Cell growth rate reduction: EC10 (0-72h) equal to 15 mg/l (95% confidence limits 7 to 30); EC50 (0-72h) equal to 82 mg/l (95% confidence limits 39 to 170).

Cell growth rate reduction: EC10 (24-72h) equal to 15 mg/l (95% confidence limits 7 to 31); EC50 (24-72h) equal to 39 mg/l (95% confidence limits 19 to 81).

Reliability : (1) valid without restriction
15.03.2000 (12)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO OTHER NON-MAMM. TERRESTRIAL SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Species	:	rat
Strain	:	
Sex	:	male/female
Number of animals	:	10
Vehicle	:	other
Value	:	> 500 mg/kg bw
Method	:	other
Year	:	1971
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	5 male and 5 female Sprague-Dawley rats with an average body weight of 191 grams were fasted for approximately 18 hours prior to dosing. The Surfynol 104 was prepared as a 5% solution in hydrous alcohol. Each rat received a dose volume of 10 ml/kg of body weight. The animals were observed daily post-dose for 14 days.
Result	:	All animals survived, showed no abnormal clinical signs and gained weight. Gross necropsy did not reveal any test material-related pathological changes.
Source	:	APCI (EXT-86/020) / Foster D. Snell Inc. Biological Science Laboratories
Reliability	:	(2) valid with restrictions Study pre-dates GLPs.

13.12.2001 (3)

5.1.2 ACUTE INHALATION TOXICITY

Type	:	LC50
Species	:	rat
Strain	:	
Sex	:	male/female
Number of animals	:	10
Vehicle	:	water
Exposure time	:	1 hour(s)
Value	:	> 20 mg/l
Method	:	other
Year	:	1971
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	5 male rats (average weight 176 grams) and 5 female rats (average weight 211 grams) were placed in a 306 liter chamber. The Surfynol 104 was prepared as a 5% aqueous solution. An air flow of five liters per minute was introduced into the chamber. The test solution was aerosolized to provide a concentration of greater than 20 mg of mist per liter of chamber air over the one-hour period. The test atmosphere was not analyzed. The animals were observed daily for 14 days.
Result	:	All animals survived. Ocular and nasal irritation as well as a reduction in spontaneous activity was noted in all

animals immediately following the one-hour exposure. All animals returned to normal within 3 hours. One male and one female were autopsied at random. Gross necropsy did not reveal any test material-related pathological changes.

Source : APCI (EXT-86/020) / Foster D. Snell Inc. Biological Science Laboratories

Reliability : (2) valid with restrictions
Study pre-dates GLPs

13.12.2001 (3)

5.1.3 ACUTE DERMAL TOXICITY

Type : LD50
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Value : > 2000 mg/kg bw
Method : OECD Guide-line 402 "Acute dermal Toxicity"
Year : 1993
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Source : APCI (EXT-94/012) / Notox B.V.
Test substance : Surfynol 104 batch # 21902
Reliability : (1) valid without restriction
21.09.1999 (6)

Type : LD50
Species : rabbit
Strain : New Zealand white
Sex : no data
Number of animals : 6
Vehicle :
Value : > 1000 mg/kg bw
Method : other
Year : 1971
GLP :
Test substance :
Method : 6 New Zealand White rabbits with an average body weight of 3 kilograms were selected for dosing. The skin of the trunk was clipped free of hair exposing an average surface area of approx. 240 square centimeters. The neat Surfynol 104 (1000 mg/kg) was applied to the intact skin site. The entire trunk of each animal was then encased in a plastic sleeve to insure continuous contact of the test material with the skin for a 24-hour period. The sleeve was removed after 24-hours and the animals were observed daily post-dose for 14 days.

Source : APCI (EXT-86/020) / Foster D. Snell Inc. Biological Science Laboratories
Test substance : Surfynol 104 was applied neat.
Reliability : (2) valid with restrictions
06.11.2001 (3)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

Species	:	rabbit
Concentration	:	
Exposure	:	Semiocclusive
Exposure time	:	4 hour(s)
Number of animals	:	3
PDII	:	
Result	:	
EC classification	:	irritating
Method	:	OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year	:	1993
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	Moderate to severe erythema and slight edema in the animals. Reduced flexibility of the treated skin was noted in two animals 72 hours after exposure only. The skin irritation had resolved within 21 days after exposure in all animals. No corrosive effect occurred on the skin in any of the three rabbits. Primary irritation index of 4.3 (moderately irritating) when melted and applied to the intact skin.
Source	:	APCI (EXT-94/010) / NOTOX
Reliability	:	(1) valid without restriction

06.11.2001 (5)

Species	:	rabbit
Concentration	:	
Exposure	:	Semiocclusive
Exposure time	:	4 hour(s)
Number of animals	:	3
PDII	:	
Result	:	slightly irritating
EC classification	:	not irritating
Method	:	OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year	:	1994
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	The test article was weighed and 0.5 g was moistened with distilled water (made pasty) to ensure good contact with the skin. The resultant paste was applied to the clipped site in a manner allowing even distribution of the test article over the 6 centimeter squared test site. The test site was then covered with a semiocclusive dressing.
Result	:	Erythema, slight at 30 - 60 minutes after patch removal, was absent to slight at 24 hours and absent at 48 and 72 hours. Edema, was absent at all observation intervals. There were no abnormal physical signs noted during the observation period. Primary Irritation Index of 0.17 (mildly irritating) when applied to the intact skin.

13.12.2001

5.2.2 EYE IRRITATION

Species	:	rabbit

Concentration	:	
Dose	:	0.1 ml
Exposure Time	:	
Comment	:	
Number of animals	:	9
Result	:	highly irritating
EC classification	:	irritating
Method	:	other
Year	:	1998
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	EPA/TSCA Health Effects Testing Guidelines, 40 CFR Part 798.45.00.
Remark	:	Nine healthy New Zealand White rabbits, free from evidence of ocular irritation and corneal abnormalities, were dosed. Surfynol 104 (0.1 ml) was placed into the conjunctival sac of one eye of each rabbit. Six eyes remained unwashed. Three eyes were washed with lukewarm water for one minute, 30 seconds postdose. The eyes were examined and scored by the Draize technique at one hour and at 24, 48, and 72 hours postdose. In order to determine reversibility, the eyes were examined again on Days 7, 14, and 21. Sodium fluorescein was used to determine corneal effects following the 24-hour scoring interval.
Result	:	Unwashed eyes: Corneal opacity, noted in 6/6 eyes, persisted to Day 21 in 3/6 eyes. Iritis, noted in 6/6 eyes, cleared by Day 7. Conjunctival irritation, noted in 6/6 eyes, cleared by Day 14. Washed eyes: Corneal opacity, noted in 3/3 eyes, cleared by Day 14. Iritis, noted in 3/3 eyes, cleared by Day 7. Conjunctival irritation, noted in 3/3 eyes, cleared by Day 14.
Source	:	APCI (EXT-98/164) / MB Research
Reliability	:	(1) valid without restriction

21.09.1999 (9)

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

Species	:	rat
Sex	:	male/female
Strain	:	Long-Evans
Route of admin.	:	oral feed
Exposure period	:	28 days
Frequency of treatment	:	continuous
Post obs. period	:	
Doses	:	0, 625, 1250, 2500, and 5000 ppm
Control group	:	yes, concurrent no treatment
NOAEL	:	= 5000 ppm
Method	:	other
Year	:	1977

GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Rats were assigned to groups by body weight. Each group was composed of 6 rats of each sex. The rats were approximately 6-7 weeks of age at the start of the test. Test diets were made up on a weekly basis. Statistical analysis of the body weight and food consumption data was performed using the F-test and the Student's t-test.
Result	:	Mortality, physical observations, body weight, and food consumption data, as well as gross necropsy observations did not reveal any adverse effects considered to be attributable to the administration of Surfynol 104 at any of the dose levels. NOEL=5000 ppm (high-dose).
Source	:	APCI (EXT-77/016) / Biodynamics, Inc.
Reliability	:	(2) valid with restrictions Study pre-dates GLPs

21.09.1999 (2)

Species	:	dog
Sex	:	male/female
Strain	:	Beagle
Route of admin.	:	other
Exposure period	:	130 days
Frequency of treatment	:	daily
Post obs. period	:	
Doses	:	0, 200, 250, and 300 mg/kg/day
Control group	:	yes
LOAEL	:	= 200 mg/kg
Method	:	other
Year	:	1979
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	32 pure-bred Beagles (16 of each sex) weighing approx. 4.6 to 9.0 Kg and being 4-5 months of age were quarantined for 21 days and then randomized into four groups each containing 4 males and 4 females. Randomization was performed in such a way that no same sex siblings were in the same group and an even distribution of body weights was obtained. All groups received 350 grams of food per day. All dosing was done using ¼ ounce gelatin capsules. Capsule administration followed feeding by approximately one hour. The control animals received capsules of granulated table sugar. The low-dose group received 50 to 200 mg of Surfynol 104 per kg of body weight per day. The mid- and high-dose group received 50 to 300 mg/kg/day. The mean weekly body weight of each group was used to calculate the dose. Doses were calculated separately for each sex. Statistical analysis of the body weight, food consumption, clinical chemistry, hematology and organ weight data was performed using the Student t test.
Remark	:	The test material was administered orally to beagle dogs in gelatin capsules at dose levels of 200, 250 and 300 mg/kg/day for 91 days. Because the dogs had to be gradually acclimated from 50 mg/kg/day to higher dose levels of SURFYNOL 104 to avoid vomiting, the total test period was 130 days.

Result	:	All dogs survived for the duration of this study with few clinical signs. Occasional dogs in the mid- and high-dose groups exhibited sporadic compound-related neurologic disturbances (convulsions and tremors) during the study. All other observations, including feed consumption, body weight gains, organ weights (except liver), clinical chemistries, hematology, urinalysis, gross pathology, and histology were judged to reflect no compound-related/ biologically significant changes. This study did not establish a no-effect level (NOEL) of Surfynol 104 in dogs, since mean liver weights and liver-to-body weight ratios in all Surfynol 104-treated groups were higher than in corresponding control groups. However, since no historical abnormalities were observed in these livers, the liver enlargement was judged to be due to hyperplasia of the hepatic endoplasmic reticulum, where xenobiotic/drug metabolizing enzymes are located. These common adaptive liver changes are generally reversible, after test compound exposure is discontinued.
Source	:	APCI (EXT-94/090) / Pharmacopathics Research Laboratories
Test substance	:	Surfynol 104 lot # 2910-109 (purity 100%)
Reliability	:	(2) valid with restrictions

13.12.2001 (7)

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Ames test
System of testing	:	Salmonella typhimurium strains TA1535, TA1537, TA98, TA100, and E-coli strain WP2(uvrA).
Concentration	:	0, 10, 50, 100, 500, 1000, and 5000 ug/plate
Cycotoxic conc.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	OECD Guide-line 471 "Genetic Toxicology: Salmonella thyphimurium Reverse Mutation Assay"
Year	:	1999
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Reliability	:	(1) valid without restriction

15.03.2000 (15)

Type	:	Cytogenetic assay
System of testing	:	CHO Cells
Concentration	:	19.5, 39.1, 78.1-78.3, 156.3, 312.5, 1250, and 3500
Cycotoxic conc.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	OECD Guide-line 473 "Genetic Toxicology: In vitro Mammalian Cytogenetic Test"
Year	:	1999
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Reliability	:	(1) valid without restriction

15.03.2000 (16)

5.6 GENETIC TOXICITY 'IN VITRO'

5.7 CARCINOGENITY

5.8 TOXICITY TO REPRODUCTION

Type	:	One generation study
Species	:	rat
Sex	:	male/female
Strain	:	Sprague-Dawley
Route of admin.	:	oral feed
Exposure period	:	variable
Frequency of treatment	:	continuous
Premating exposure period		
Male	:	None
Female	:	None
Duration of test	:	135 days
Doses	:	0, 500, 1000, and 2000 mg/kg/day
Control group	:	yes, concurrent no treatment
NOAEL Parental	:	= 500 mg/kg bw
NOAEL F1 Offspr.	:	= 500 mg/kg bw
Method	:	other
Year	:	1979
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Ten male and twenty female sexually mature rats were randomly assigned to each group. Males were sacrificed following the 20th day of breeding and females were sacrificed when their litters were weaned at 21 days of age. Animals were fed their respective diets from the start of cohabitation until their scheduled sacrifice. The weanlings were randomized within their respective groups and carried on the same dose levels as their parents for 91 days. Test diets were prepared weekly. Analytical monitoring of the test diets was performed. Statistical analysis of the body weight, food consumption, clinical chemistry, and hematology data was performed using the Student's t-test.
Result	:	The only pertinent findings observed in the Fo parents were: a slight decrease in the mean weaning weight of both male and female pups of the high-dose group, a slight decrease in lactation indices of the high-dose group, decreased body weight and feed consumption of the high-dose female group and normal histology of the reproductive organs in the Fo parents. Fertility, viability and gestation indices were not affected. In the reproduction phase of this experiment there was a toxic effect at the 2,000 mg/kg/day level, a borderline effect at the 1,000 mg/kg/day level and no effect at 500 mg/kg/day. The following pertinent findings were observed in the F1a rats: slight decrease in the mean rate of body weight gain in both sexes at the mid- and high-dose (there was also a significant decrease in this parameter in the low-dose male group during the first eight weeks), normal mean

hematological findings, clinical chemistry findings, and urinalysis findings after 91 days on test, significant increase in the absolute and relative liver weights of both sexes at the mid- and high-dose, corresponding histopathology of the liver showing mild to moderate centrilobular cloudy swelling of hepatocytes of the mid- and high-dose rats. Surfynol 104, when fed to rats under the conditions of this experiment, showed no effect at 500 mg/kg/day but did have a toxic effect in the F1a generation at >1,000 mg/kg/day.

Source : APCI (EXT-97/005) / Pharmacopathics Research Laboratories
Test substance : Surfynol 104 lot # 2910-109 (purity 100%)
Reliability : (1) valid without restriction
21.09.1999 (8)

5.9 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.10 OTHER RELEVANT INFORMATION

5.11 EXPERIENCE WITH HUMAN EXPOSURE

(1) APCI (EXT-00/001) / NOTOX

(2) APCI (EXT-77/016) / Biodynamics, Inc.

(3) APCI (EXT-86/020) / Foster D. Snell Inc. Biological Science Laboratories

(4) APCI (EXT-92/040) / Commonwealth Technology, Inc.

(5) APCI (EXT-94/010) / NOTOX

(6) APCI (EXT-94/012) / Notox B.V.

(7) APCI (EXT-94/090) / Pharmacopathics Research Laboratories

(8) APCI (EXT-97/005) / Pharmacopathics Research Laboratories

(9) APCI (EXT-98/164) / MB Research

(10) APCI (EXT-99/101) / NOTOX

(11) APCI (EXT/00-007) / NOTOX

(12) APCI (EXT/00-030) / NOTOX

(13) APCI (EXT/00-059) / NOTOX

(14) APCI (EXT/99-007) / NOTOX

(15) APCI (EXT/99-078) / SRI International

(16) APCI (EXT/99-091) / SRI International

7.1 END POINT SUMMARY

7.2 HAZARD SUMMARY

7.3 RISK ASSESSMENT

Remark : Potential for Worker Exposure During 2,4,7,9-tetramethyl-5-decyne-4,7-diol Manufacturing

2,4,7,9-tetramethyl-5-decyne-4,7-diol is produced by the reaction of acetylene and ketone. The crude product stream is continuously extracted from the reactor and then batch distilled. Once final product is obtained from the distillation, the product is blended with solvents to make one of several liquid products, or converted to polyethylene glycol ether surfactants via ethoxylation. The products can be drummed, loaded into totes, or loaded into trailers for bulk customer shipments. Workers in the drumming operation, which is ventilated mechanically, wear personal protective equipment including gloves, coveralls, and eye protection.

Most 2,4,7,9-tetramethyl-5-decyne-4,7-diol sold for surfactant applications is provided to industrial users. Because the surfactant is a difficult-to-handle, waxy solid, nearly all of these users purchase the product in 55-gallon drums or bulk quantities dissolved in a suitable solvent. The solvent enables ready formulation into a coating, ink, or adhesive and minimizes worker contact with the surfactant itself. Workers who make inks, coatings, or adhesives generally transfer the surfactant into day tanks where it is subsequently delivered into mixing units without additional need for human intervention. Such formulated products contain very low levels of 2,4,7,9-tetramethyl-5-decyne-4,7-diol.

Risk Management

The known toxicity information about 2,4,7,9-tetramethyl-5-decyne-4,7-diol suggests the acute effects of greatest concern are skin and eye irritation. Personal protective equipment recommendations for these effects are believed to be sufficient to protect against low levels of dermal exposure as well. 2,4,7,9-tetramethyl-5-decyne-4,7-diol has a low vapor pressure and low acute inhalation toxicity so unusual ventilation requirements are not required.

Based on the known toxicological endpoints, the following personal protection / exposure controls are recommended:

Eye protection: Splash-proof eye goggles. In emergency situations, use eye goggles with a full-face shield.

Hand protection: Neoprene rubber gloves. Nitrile rubber gloves. Insulated gloves such as thermal lined rubber when handling hot material.

Ventilation: Well-ventilated workplace.

Protective clothing: Long sleeved clothing.

Work and hygienic practices: Provide readily accessible eye wash stations and safety showers. Wash at the end of each work shift and before eating, smoking or using the toilet.

13.12.2001